

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.53×10^{-14} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.55×10^{-1}

Confidence level: 6.35×10^{-1}

Nearest Neighbors from the Training Set

Image not found

1,1,2,2-Tetrachloroethane

Measured: 2.50×10^{-13}

Predicted: 1.03×10^{-13}

Image not found

1,1,1,2-Tetrachloroethane

Measured: 1.80×10^{-14}

Predicted: 4.29×10^{-14}

Image not found

2,2,2-Trichloroethanol

Measured: 2.45×10^{-13}

Predicted: 2.56×10^{-13}

Image not found

Methane, trifluoromethoxy-

Measured: 2.14×10^{-14}

Predicted: 1.62×10^{-14}

Image not found

1,2-Dichloro-1,1-difluoroethane

Measured: 1.60×10^{-14}

Predicted: 1.99×10^{-14}